Macromolecular Crystallography Software

This page describesto all software packages that are available at GM/CA. Supported programs and packages are regularly updated (usually within 2-3 months of the version release) and thoroughly tested in the beamline computer environment. Unsupported programs are also available to the users, but support staff cannot guarantee that they are up to date, or correctly configured and will not provide help to fix problems occrring while running these programs.

Data Processing

- Mosflm: Auto indexing, Strategy and Integration A program for visualization, indexing and integrating single crystal diffraction data from area detectors. Supported
- Scala This program scale together multiple observations of reflections, and merges multiple observations into an average intensity. Supported
- Denzo/Scalepack Programs for processing (index, integrate and scales) single crystal diffraction data. Supported
- HKL2000 The HKL2000 suite of programs package contain Denzo, XdisplayF, Scalepack, STRAT (program for strategy and simulation). Supported
- Labelit A new robust autoindexing program. Supported

Phasing and Refinement

- SOLVE & RESOLVE SOLVE program can carry out steps of macromolecular structure determination from scaling of the data sets to the calculation of an electron density map automatically. The companion program RESOLVE improves the electron density maps obtained from SOLVE or other phasing programs. Supported. We also update the MAD data processing scripts located in users "templates" directory.
- SHELX SHELX is a set of programs for crystal structure determination from single-crystal diffraction data. This suite can also perform structure refinement. Supported (shelxc-e)
- SnB SnB program is based on Shake-and-Bake, a dual-space direct-methods procedure for determining crystal structures from X-ray diffraction data. Unsupported
- SHARP & autoSHARP This progarm can do different types of phasing methods. Unsupported
- PHASES Program package to compute phase angles for diffraction data from macomolecular crystals. Unsupported
- CNS Performs phasing, density modification, and refinement of macromolecules. Unsupported
- CCP4 package CCP4 suite is a set of programs which communicate via standard data files. It has several programs for data manipulation, phasing, and refinement of macromolecules. Supported
- ARP/wARP ARP/wARP is a software suite for improvement and objective interpretation of crystallographic electron density maps. It also performs automatic tracing and refinement of macromolecular models. Unsupported

Model Building and Molecular Graphics

- O This is a program for model building using electron density maps and model manipulation. Supported
- XtalView A Complete Package for Solving a Macromolecular Crystal Structure. Unsupported

- Turbo Frodo Program for model building using electron density maps and model manipulation. Unsupported
- PyMOL PyMOL program is a molecular graphics program with high-quality rendering, animations and other common molecular graphics activities. Unsupported
- MolScript MolScript is a program for displaying molecular 3D structures in both schematic and detailed representations. Unsupported
- RasMol A molecular graphics program inteded for the visualisation of macromolecules and small molecules. Unsupported
- Raster3D A set of tools for generating high quality raster images for proteins or other molecules. Unsupported
- POV-Ray The Persistence of Vision Raytracer (POV-Ray) is a high-quality tool for creating three-dimensional graphics. Unsupported
- LIGPLOT LIGPLOT automatically generates schematic diagrams of protein-ligand interactions from the 3D coordinates in a PDB file. Unsupported
- Ribbons Graphics program to display molecular models and for drawing molecular pictures. Unsupported

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